REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-06-0145

1. REPORT DATE 03-01-2006

2. REPORT TYPE Final

3. DATES COVERED May 2004 – June 2005

4. TITLE AND SUBTITLE

Development of a Multiprocessor Linux Parallel Cluster for Magnetohydrodynamic Computations

5a. CONTRACT NUMBER

5b. GRANT NUMBER FA9550-04-1-0398

5c. PROGRAM ELEMENT NUMBER

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/NA
Dr. John Schmisseur
875 North Randolph Street
Suite 325 , Room 3112
Arlington , VA 22203-1768

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; – Distribution A –
distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The objective of the funded program was to establish a Beowulf-class cluster system to support DoD sponsored research programs conducted at Wichita State University. Currently, a comprehensive research program in support of the magnetohydrodynamics (MHD), hypersonic activities of AFOSR in search of innovative and integrated hypersonic flowfield simulation is underway. Furthermore, preparation of several proposals in high speed flows, flow control, turbulence and MHD is underway and one such proposal has been submitted to DoD. These research programs are computationally intensive in terms of storage requirements and CPU time. Current computational resources for our efforts are inadequate. The available computational resources are shared by all researchers and therefore, the turn-around-time for computationally intensive efforts is extremely slow. The established cluster computer system has eliminated this problem and allows sufficient progress of our research activities. Similar systems have proven to be cost effective and efficient. The system can be upgraded due to the use of commodity off-the-shelf technology implemented in the cluster system. Recently, a similar system was established at the US Air Force Academy for their computationally intensive jobs. The results in terms of efficiency have been excellent. The established cluster computer system has already proven a valuable tool in term of efficiency and its capabilities.

15. SUBJECT TERMS Magnetohydrodynamic , Turbulence , Hypersonic , Computational Fluid Dynamics , Large Eddy Simulations

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Klaus A. Hoffmann
a. REPORT	b. ABSTRACT	c. THIS PAGE		18	19b. TELEPHONE NUMBER *(include area code)* (316) 978-6327

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

DEVELOPMENT OF A MULTIPROCESSOR LINUX PARALLEL CLUSTER FOR MAGNETOHYRODYNAMIC COMPUTATIONS

AFOSR GRANT # FA9550-04-1-0398

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Abstract

The objective of the funded program was to establish a Beowulf-class cluster system to support DoD sponsored research programs conducted at Wichita State University. Currently, a comprehensive research program in support of the magnetohydrodynamics (MHD), hypersonic activities of AFOSR in search of innovative and integrated hypersonic flowfield simulation is underway. Furthermore, preparation of several proposals in high speed flows, flow control, turbulence and MHD is underway and one such proposal has been submitted to DoD. These research programs are computationally intensive in terms of storage requirements and CPU time. Current computational resources for our efforts are inadequate. The available computational resources are shared by all researchers and therefore, the turn-around-time for computationally intensive efforts is extremely slow. The established cluster computer system has eliminated this problem and allows sufficient progress of our research activities. Similar systems have proven to be cost effective and efficient. The system can be upgraded due to the use of commodity off-the-shelf technology implemented in the cluster system. Recently, a similar system was established at the US Air Force Academy for their computationally intensive jobs. The results in terms of efficiency have been excellent. The established cluster computer system has already proven a valuable tool in term of efficiency and its capabilities.

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Chapter 1

Introduction

The concepts of flow control and enhancement of hypersonic vehicles by the application of a magnetic field have recently gained considerable attention. Several advanced concepts for propulsion and flow control have been proposed and to some extent have been demonstrated primarily based on analytical and numerical solutions of the governing equations. In parallel studies, some experimental investigations have also been conducted.

In order to develop optimization processes for design and performance analyses, several critical issues must be addressed and resolved. The complexity of the flowfield is of course due to chemical and thermal equilibrium/non-equilibrium, transition, turbulence, and interaction of the applied/induced magnetic field with the flowfield. The difficulty is compounded because most of these physical phenomena occur simultaneously and the physics and the processes involved are poorly understood. Flow control and propulsion therefore have emerged as critical problems for design and performance of hypersonic vehicles and propulsion systems.

With the advances in computer technology and progress in higher-order numerical schemes, a new tool referred to as Computational Fluid Dynamics (CFD) has emerged. Over the past three decades, Computational Fluid Dynamics has reached a level of maturity that is now possible to compute flowfields associated with complex geometries such as aircraft, turbomachinery, automobiles and missiles.

Currently, a computational code is being developed to provide a tool for design and performance analyses of magnetohydrodynamics (MHD) of high-speed flows. Each segment of the computer code is validated by comparison of the numerical solution with the available analytical solutions, other numerical solutions reported in the literature, and experimental data when available [1-3]. The completed MHD code is an integrated computational tool for steady or unsteady flows with options for chemical models (equilibrium/non-equilibrium) [4,5], turbulence (options for 5 different models) [6,7,8], and three-dimensional geometries [9,10]. To address realistic design and analyses concerns, such a sophisticated code which includes all physical parameters is necessary. However, including all of the required physics in the computation is computer intensive, both in terms of storage requirement and CPU time. In the past, the computations were performed on the HYDRA (Origin 2000) machine at Wichita State University (WSU). However, this resource was shared by all researchers at WSU, and therefore, turn around time for computationally intensive jobs was extremely slow. To overcome this impediment to the MHD research program, the purchase of a cost effective cluster system operating in parallel was proposed. Recently, a similar system has been set up at the USAFA for their computationally intensive jobs. The result in terms of efficiency is excellent.

Even though computational resources at Wichita State University have been improved over the last several years, there had been an explosion of the number of faculty and student users. At the present time, computer facilities are saturated, and long delays on computationally intensive jobs hinder progress on our research activities. The established cluster computer system has eliminated this problem and now allows sufficient progress of our research activities. A short description of computationally intensive projects currently underway is provided in the following chapter.

Chapter 2

Research Activities

2.1 An Integrated Computational Tool for Hypersonic Flow Simulation

In recent investigations, several physical phenomena including thermal and chemical equilibrium and/or non-equilibrium, transition/turbulence, and MHD have been identified which must be integrated and collectively used to predict hypersonic flowfields. A proposal to develop such a tool for design and performance analysis and ultimately for an optimization process was funded under the DEPSCoR initiative and administered by the Air Force Office of Scientific Research.

The research activities are in line with the New World Vista Vision for Air Vehicle and Propulsion, and in fact will specifically address the shortcomings identified by the Air Force. It is anticipated that the integrated code will identify and address issues with regard to wave and skin-friction drag reduction, heat transfer, and turbulence under the influence of a magnetic field.

The currently ongoing research program "An Integrated Computational Tool for Hypersonic Flow Simulations" consists of the following tasks:

1. Formulation of a unified computational approach for fluid, MHD, chemistry equations and turbulence models- the development will include the numerical analysis framework for determining the resolution characteristics, error estimates, stability and efficiency
2. Determination of eigenvectors of the system of equations necessary for the development of numerical schemes and TVD models
3. Formulation and implementation of perfectly matched layer, or sponge layer, for far-field boundary conditions
4. Validation of the accuracy and efficiency of the chemical and turbulence models and the numerics for
   a. Chemical models
      - Equilibrium [11]
      - Non Equilibrium - Five species model, 17 chemical reactions [12]
   b. Turbulence models
      - Zero-equation model - Baldwin-Lomax zero-equation turbulence model [13]
      - One-equation models
        * Baldwin-Barth one-equation turbulence model [14]
        * Spalart-Allmaras one-equation turbulence model [15]
      - Two-equation models
        * $k-\varepsilon$ two-equation turbulence model [16]
        * combined $k-\varepsilon/k-\omega$ two-equation turbulence model [17]
      - Modification to turbulence model to include effect of magnetic field
5. Integration of the individual components to form the Integrated Hypersonic Magnetohydrodynamic Computation Tool (IHMCT)

6. Validation of IHMCT for Hypersonic flows over simple geometries such as compression corner and channel flows with the influence of magnetic field
7. Application of IHMCT for inlet of hypersonic vehicles for flow characterization, flow physics and optimization.

Tasks 1 through 3 are completed and tasks 4 through 7 are in progress. The results of the completed and ongoing tasks have been reported in several publications [1-10]. The progress of the program, and in particular in the implementation of tasks 5 through 7, was slow due to availability of computer resources. To remedy this difficulty, the purchase of a clustered computer system was proposed. With the establishment of the new cluster computer system sufficient resources are now available to allow adequate progress of the ongoing program and future programs.

2.2 Direct Numerical Simulation

A research program leading to Direct Numerical Simulation (DNS) of compressible transitional and turbulent flow with the effect of magnetic and electric fields at moderate Reynolds numbers is under development.

The DNS approach is an "exact method" in the sense that the original governing equations are solved without any modifications, or filtering process. If the error introduced by the numerical scheme can be evaluated or controlled, DNS can provide high quality results, similar to those of an experiment. Note that the equations are solved on an extensive number of locations in the flow field, allowing the collection of a large amount of information that would be impossible to obtain from an experiment. For example, it is possible to numerically "probe" the flow very close to a solid surface, whereas it is relatively difficult to do so experimentally. DNS also provides results in the entire flow field at a given time level, which is identical for all locations (necessary condition to evaluate the cross correlation terms). This requirement is very difficult to meet in an experiment.

Most of the previous work in Direct Numerical Simulation of compressible unsteady Navier-Stokes equations has been limited to simple geometries (e.g., flat plates and channel flows, etc.) and relatively low Reynolds numbers (Re). The principal reasons for this scarcity of DNS results are that the number of grid points required for 3-D DNS scales as $(Re)^{9/4}$, and therefore, the computation at Re $\cong$ 1 million have been beyond the scope of available computers and secondly, the globally accurate spectral methods have not been easily extendible to complex geometries. With the advent of parallel computing, it is now feasible to perform a DNS for transitional and turbulent flows. However, the algorithms employed on body-fitted curvilinear grids must be such that they retain the accuracy of spectral methods and are free from the phenomenon known as aliasing. The proper treatment of far-filed boundary conditions on a finite-computational domain is also very critical for accurate DNS simulation of compressible MHD flows.

In the current research, a sixth-order compact discretization will be employed for the spatial terms on non-uniform curvilinear grids. Periodicity will be assumed in the spanwise-direction, again using sixth-order compact differences. An eight-order compact dissipation operator will be added to annihilate the physically nonrealizable spurious modes which are the artifact of numerical discretization. A novel treatment of the far-field boundary conditions based on the modal analysis of the similarity form of the Navier-Stokes equations will be implemented.

This technique assures that all incoming modes in the computational domain are annihilated (truly non-reflecting far-field boundary condition).

It is anticipated that the innovative computational approach of the current research program along with the Beowulf cluster computers will result in a compressible DNS code applicable for transitional and turbulent MHD flow simulations at realistic Reynolds numbers (of approximately 1 million). The code will be validated against existing DNS results for fully developed turbulent channel flow and a spatially evolving boundary layer to assess its accuracy and efficiency. Finally, the validated code will be applied to simulate the transitional and turbulent MHD flows at moderate Reynolds numbers.

The current research program will consist of the following tasks:

a. Development of a compact higher order (sixth-order) numerical scheme on non-uniform curvilinear grids– the development will include the numerical analysis framework for determining the resolution characteristics, error estimates, and stability
b. Formulation and implementation of a non-reflecting far-field boundary condition such as perfectly matched layer
c. Code development and implementation on parallel computing platforms
d. Validation of the accuracy and efficiency of the algorithm by computing existing DNS test cases
    - Simulating fully developed turbulent channel flow
    - Spatially evolving boundary layer on a flat plate
    - Supersonic flow in a compression corner.
e. Application of DNS code to compute the compressible transitional and turbulent MHD flows at moderate Reynolds numbers.

To successfully accomplish tasks d and e, several million grid points will be required.

2.3 Large Eddy Simulation

The second available approach regarding turbulence is the Large Eddy Simulation (LES) [18]. Large scales are numerically computed, whereas the small scales are modeled by simple eddy viscosity models, known as Sub Grid Scale models (SGS). Large Eddy Simulation is a good compromise between the Reynolds Averaged approach (RANS) and the Direct Numerical Simulation, because it is more versatile than RANS and less costly than DNS.

In fluid mechanics, flows present a wide range of scales, both in length and in time. The accuracy of a simulation method relies on the ability to resolve all scales of motion. The large scales are more energetic and more effective in the transport process of turbulent quantities (energy and moments) and the small scales are assumed more universal than the large scales and are responsible for most of the energy dissipation. Large Eddy Simulation (LES) is able to resolve large scales of motions, whereas small scales are modeled by simple eddy viscosity models, known as Sub Grid Scale models (SGS). Algebraic models are sufficient, because the imperfections of these simple models should not greatly affect the solution. LES is less costly than DNS. In fact it typically requires less than 10% of the computer resources required for DNS.

2.4 Detached Eddy Simulation

Other hybrid methods have been developed. The Detached Eddy Simulation (DES) combines the RANS approach in regions of thin boundary layer where no separation occur, and switches to LES in regions of massive separation [19-23]. This method allows a substantial reduction of the computational cost associated with LES. Therefore, turbulent flow field can be numerically investigated within a reasonable time.

Detached Eddy Simulation is a recent hybrid method. It includes a simple turbulence model that acts as a regular RANS model in the boundary layer and switches to a Sub Grid Scale model in regions of large separation. DES is therefore more affordable than LES and is able to predict separated flows.

Each approach for the computation of turbulent flows will not be considered independent from each other. The DNS results, which require the most computer resources, will be used to improve and tailor the LES, DES, and RANS methods. DNS results should provide sufficiently accurate data that will allow the specification of transition information and calibration of closure coefficients associated with LES, DES, and RANS.

Chapter 3

Technical Approach

The funded program consisted of the following tasks:

1. Purchase of a 46 node, 92 processors Linux clusters
2. Installation of software, including Linux Red Hat, Absoft Fortran Compiler, Portland Group Compiler
3. In addition to the in house codes developed for MHD, acquire the commercially available code Cobalt 60 and develop modulars for MHD applications.

Due to price reduction , and additional educational discount, we were able to purchase a 92 processor machine and all the required software within the allocated budget.

3.1 Research Infrastructure Development

The proposed research program included two key components essential to advance the research infrastructure at the Wichita State University. One element is the training of graduate students in computational schemes and parallel computing and the second element is the development of efficient and cost effective computational resources to conduct the proposed computational developments in support of various DoD research programs. Both of these elements has strengthen with the establishment of the cluster machine.

3.2 Research and Education Training of Students

One of the key components of the program was to train graduate students for research in parallel computing, turbulent flow simulation and magnetohydrodynamics. There is currently a significant amount of research activities in the areas of turbulence, chemistry, parallel computing, and MHD by the principal investigator. The funded research project has substantially enhanced the graduate research program in the computation of high speed, turbulent flows, with imposed and/or induced electromagnetic fields.

Several courses are currently offered in the department of aerospace engineering in basic and advanced computational fluid dynamics. These courses provide the foundations for numerical schemes, grid generation methods, boundary conditions, etc. for solving multidimensional partial differential equations. In addition, several courses in turbulence and hypersonics have been recently developed, which provide the necessary background for the physical aspects of the problems under consideration.

3.3 Beowulf Cluster

Beowulf Cluster systems offer a cost-effective alternative to traditional supercomputers [24]. Their cost-effectiveness is due to the exclusive use of components that are already available for large markets. The typical price/performance ratio is about ten times lower than other traditional supercomputers such as Cray TSE or IBM SP3. Furthermore, the use of off-the-shelf components provides a greater flexibility to configure and upgrade the system. Beowulf Clusters have become popular over the last several years by integrating low cost or no cost system softwares. It typically operates on the freely distributed Linux operating system.

Chapter 4

Program Management and other Information

4.1 Team Organization

The principal investigator for this project was Dr. Klaus Hoffmann, Professor of Aerospace Engineering at Wichita State University. He had both the technical and managerial responsibility for the project.

4.2 Existing Related Activities

The principal investigator, along with several graduate students are currently engaged in a number of research activities in the field of computational fluid dynamics, and MHD. In particular, (1) numerical simulation of compressible, high speed turbulent flows including jet exhaust flows, shock/boundary layer interaction, and shear layers, (2) development of robust, efficient, and accurate schemes for MHD computations, (3) modifications of turbulence models to improve their prediction capabilities, and (4) hypersonic flowfield computations including chemistry effects.

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Appendix A : Details of the 92 Processor Cluster computer

GROUP: 1	QUANTITY: 1
Base Unit:	PowerConnect 3348, 48 Port FE Stackable Managed Switch,2 GbECombo Ports (221-3116)
	Type 3 Contract - Next Business Day Parts and Labor On-Site Response, Initial Year (950-1610)
	Type 3 Contract - Next Business Day Parts and Labor On-Site Response, 2YR Extended (950-1612)
	DECLINED CRITICAL BUSINESS CRITICAL SERVER OR STORAGE SUPPORT PACKAGE-CALL YOUR DELLSALES REP IF UPGRADE NEED (960-1305)

GROUP: 2	QUANTITY: 1
Base Unit:	3.6GHz/1MB Cache, Xeon, 800MHzFront Side Bus for PowerEdge 2850 (221-5966)
	3.6GHz/1MB Cache, Xeon, 800MHzFront Side Bus 2nd processor for PowerEdge 2850 (311-3945)
	4GB DDR2 400MHz (2X2GB), Dual Ranked DIMMs (311-3593)
	No Keyboard Option (310-3281)
	No Monitor Option (320-0058)
	Riser,ROMB,PCI-X,PE2850 (320-3977)
	2X36GB,U320,SCSI,1IN 10K PE2850 (341-1551)
	Embedded RAID - PERC4 Embedded Integrated (341-1506)
	1.44MB Floppy Drive (341-1308)
	Red Hat Enterprise Linux AS v33Yr RH Network Subscription No Factory Install,Drop-in-BoxW/Documentation and Media (420-4250)
	Mouse Option None (310-0024)
	Dual On-Board NICS ONLY (430-8991)
	24X IDE CD-ROM (313-2700)
	Bezel for PE2850 (313-2693)
	2+4 Split Backplane Daughtercard (311-3951)
	Electronic Documentation and OpenManage CD Kit, PE2850 (310-5474)
	146GB,U320,SCSI,1IN 10K,PE2850 (341-1306)
	MR1R5, ROMB RAID 1/RAID 5 Drives attached to PERC4ei PE2850 (341-1363)
	Rack Chassis w/Rapid Rails forDell, HPQ or other Square HoleRacks, PE2850 (310-5462)
	Premier Enterprise Support - Gold - Advanced Software Support Quantity 3 Resolutions (950-0117)
	Premier Enterprise Support Service Gold Welcome Letter (310-3785)
	Premier Enterprise On Demand Engineer Dispatch Severity 1 Three Years (970-0237)
	Type 2 Contract Same Day 4HR Parts and Labor On-Site Response,Initial Year (902-4600)
	Type 2 Contract Same Day 4HR Parts and Labor On-Site Response,Two Years (902-3262)

	Premier Enterprise Support - Gold - Premium Services, 3 Years (902-7352)
	On-Site Installation Declined (900-9997)
	OpenManage Server Subscription4 Editions, 1 Year (902-9879)
	Redundant Power Supply With Straight Cords,No Y-Cord PE2850 (310-5463)
	146GB,U320,SCSI,1IN 10K,PE2850 (341-1306)
	146GB,U320,SCSI,1IN 10K,PE2850 (341-1306)
	146GB,U320,SCSI,1IN 10K,PE2850 (341-1306)
	DPS-INF HPCC Rocks Computing Imp - 1 Week (970-0717)

GROUP: 3	QUANTITY: 1		
Base Unit:	3.6GHz/1MB Cache, Xeon 800MHz Front Side Bus for PowerEdge 1850 (221-5197)		
	No Second Processor (311-3578)		
	2GB DDR2 400MHz (2X1GB) Single Ranked DIMMs (311-3590)		
	Standard Windows Keyboard,Gray (310-1676)		
	No Monitor Option (320-0058)		
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	36GB,U320,SCSI,1IN 15K;PE1850 (341-0855)		
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	1.44MB Floppy Drive (341-0840)		
	W2K3 Server Standard Edition ACAD (420-4141)		
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	Dual On-Board NICS ONLY (430-8991)		
	Dell Remote Access Card, 4th Generation, for PowerEdge (313-2429)		
	24X IDE CD-ROM (313-2424)		
	Bezel for PE1850 (313-2421)		
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	Type 2 Contract Same Day 4HR Parts and Labor On-Site Response,Two Years (902-3262)		
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	OpenManage Server Subscription4 Editions, 1 Year (902-9879)		
	Redundant Power Supply With Dual Cords,No Y-Cord,PE1850 (310-5213)		

GROUP: 4	QUANTITY: 45		
Base Unit:	3.6GHz/2MB Cache, Xeon 800MHz Front Side Bus for PESC1425 (221-7713)		
	2nd Processor,3.6GHz / 2MB Cache,Xeon,800MHz Front Side Bus for PESC1425 (311-4827)		
	4GB DDR2 400MHz (4X1GB) Single Ranked DIMMs, PESC (311-4462)		
	No Keyboard Option (310-5017)		
	No Monitor Option (320-0058)		
	80GB 7.2K RPM SATA HDD Poweredge SC (341-1754)		
	Red Hat Enterprise Linux WS v.3,1 year RHN subscription Special HPCC Offering (420-4290)		
	NO MOUSE OPTION (320-2346)		
	CD, 650M, 24X, Internal, SAMSUNG (313-2826)		

	Bezel for PESC1425 (313-2973)
	No Hard Copy Documentation, E-Docs ONLY (410-0636)
	Motherboard SATA controller, 1Hard Drive, No RAID, PowerEdgeSC1425 (341-1522)
	Rack Chassis w/Rapid Rails forDell, HPQ or other Square HoleRacks, PEXX (310-8808)
	Type 3 Contract - Next Business Day Parts and Labor On-Site Response, Initial Year (950-7000)
	Type 3 Contract - Next Business Day Parts and Labor On-Site Response, 2YR Extended (950-7002)
	DECLINED CRITICAL BUSINESS CRITICAL SERVER OR STORAGE SUPPORT PACKAGE-CALL YOUR DELLSALES REP IF UPGRADE NEED (960-1305)
	On-Site Installation Declined (900-9997)
	HPC Cluster Compute Node Info (310-1407)

GROUP: 5	QUANTITY: 1
Base Unit:	PowerEdge 4210,Doors,Gound, 42U,PS (220-4493)
	7' Cable,8 pin,Switch Box, Mouse/Keyboard/Video (310-0973) - Quantity 2
	Type 6 Contract - Next Business Day Parts Delivery Initial Year (900-3270)
	Type 6 Contract - Next Business Day Parts Delivery 2YR Extended (900-3272)
	42U Rack Installation,Quantity1, (900-6177)
	Inside Delivery Service for Dell PowerEdge Rack System (460-0566)
	42U Rack,Interconnect Kit PS to PS (310-1282)
	16Amp, Power Distribution Unit120V, w/ IEC to IEC cords (310-1877) - Quantity 8
	15FP, 1U Rack Console with RapidRails, 15" TFT LCD, 83 key mini-kybd, U.S. (310-4226)
	Closeout Panel,2U,Black,for Dell PowerEdge Server Rack, Factory Install (310-0239)
	42U Rack,Cost Red,Side Stabilizer (310-1791)

GROUP: 6	QUANTITY: 1
Base Unit:	PowerEdge 4210,Doors,Gound, 42U,PS (220-4493)
	Type 6 Contract - Next Business Day Parts Delivery Initial Year (900-3270)
	Type 6 Contract - Next Business Day Parts Delivery 2YR Extended (900-3272)
	Install 42U Rack Quantity 1 (980-7677)
	Inside Delivery Service for Dell PowerEdge Rack System (460-0566)
	16Amp, Power Distribution Unit120V, w/ IEC to IEC cords (310-1877) - Quantity 2
	Closeout Panel,12U,Black,for Dell PowerEdge Server Rack, Factory Install (310-0244) - Quantity 2
	Closeout Panel,2U,Black,for Dell PowerEdge Server Rack, Factory Install (310-0239) - Quantity 2
	Closeout Panel,4U,Black,for Dell PowerEdge Server Rack, Factory Install (310-0241)
	42U Rack,Cost Red,Side Stabilizer (310-1791)

GROUP: 7	QUANTITY: 1
Base Unit:	8 Port Keyboard/Video/Mouse Analog Switch, 180AS (221-8096)
	8 x PS2 Server Interface Pod includes CAT5 cable (310-2835)
	Type 11 Contract - Next Business Day, Initial Year (960-4850)
	Type 11 Contract - Next Business Day, Parts,2 Year Extension (960-0322)
	DECLINED CRITICAL BUSINESS CRITICAL SERVER OR STORAGE SUPPORT PACKAGE-CALL YOUR DELLSALES REP IF UPGRADE NEED (960-1305)